Effect of Adjacent Groups on the Symmetrical CD Deformation Frequencies

Takenaka, Tohru

ABSTRACTS

Effect of Adjacent Groups on the Symmetrical CD_3 Deformation Frequencies

Tohru TAKENAKA

Nippon Kagaku Zasshi (Journal of the Chemical Society of Japan, Pure Chemistry Section), **38**, 267 (1962)

The symmetrical CD_3 deformation frequencies δ_{CD_3} of deuterated methyl compounds CD_3XH_{m-1}, CD_3XD_{m-1}, $(CD_3)_2XH_{m-2}$, $(CD_3)_2XD_{m-2}$,..... $(CD_3)_mX$ are studied in relation to the type of X atom in groups IV~VII of the periodic table, where m is the valence of X atom. The frequency variations are ascribed to changes in the deformation force constants, and can be expressed as

$$\delta_{CD_3}=317\log\left(\frac{\chi_X}{r_{CX}^2}\right)+1046$$

for almost every molecule examined. Here χ_X represents the electronegativity of X atom and r_{CX} the C-X bond length. This equation is in good agreements with the theoretical one which was derived from the results previously proposed by the author for the symmetrical CH_3 deformation frequencies of undeuterated methyl compounds, and which was obtained by taking into consideration the change of G matrix on deuteration of methyl group. Discrepancies between observed and calculated frequencies for some molecules may be attributed to the coupling of the vibration with the other modes of vibrations in the molecule.

High Pressure Synthesis of Acetic Acid from Methanol and Carbon Monoxide

Kinetic Studies on the Reaction Catalized by Phosphoric Acid

Yoshimasa TAKEZAKI, Nobuyuki SUGITA, Yukimasa FUKUI, Sachio YUASA, Minoru OSUGI and Yoshitsugu INAMORI

Journal of Japan Petroleum Institute, **3**, 708 (1960)

Kinetic studies have been made on the synthesis of acetic acid from methanol and carbon monoxide in the presence of phosphoric acid :

$$CH_3OH+CO \xrightarrow{H_3PO_4} CH_3COOH \quad \cdots\cdots(1)$$

Following results have been found out :

1) Equilibrium data :

Methanol is in equilibrium with the dehydration products *i.e.*, Me_2O and H_2O,